EFF/DOC-1144

A Comparison of diffferent Uncertainty Activation Cross-Section Data Libraries:

Application to the Prediction Uncertainty in Tritium Production

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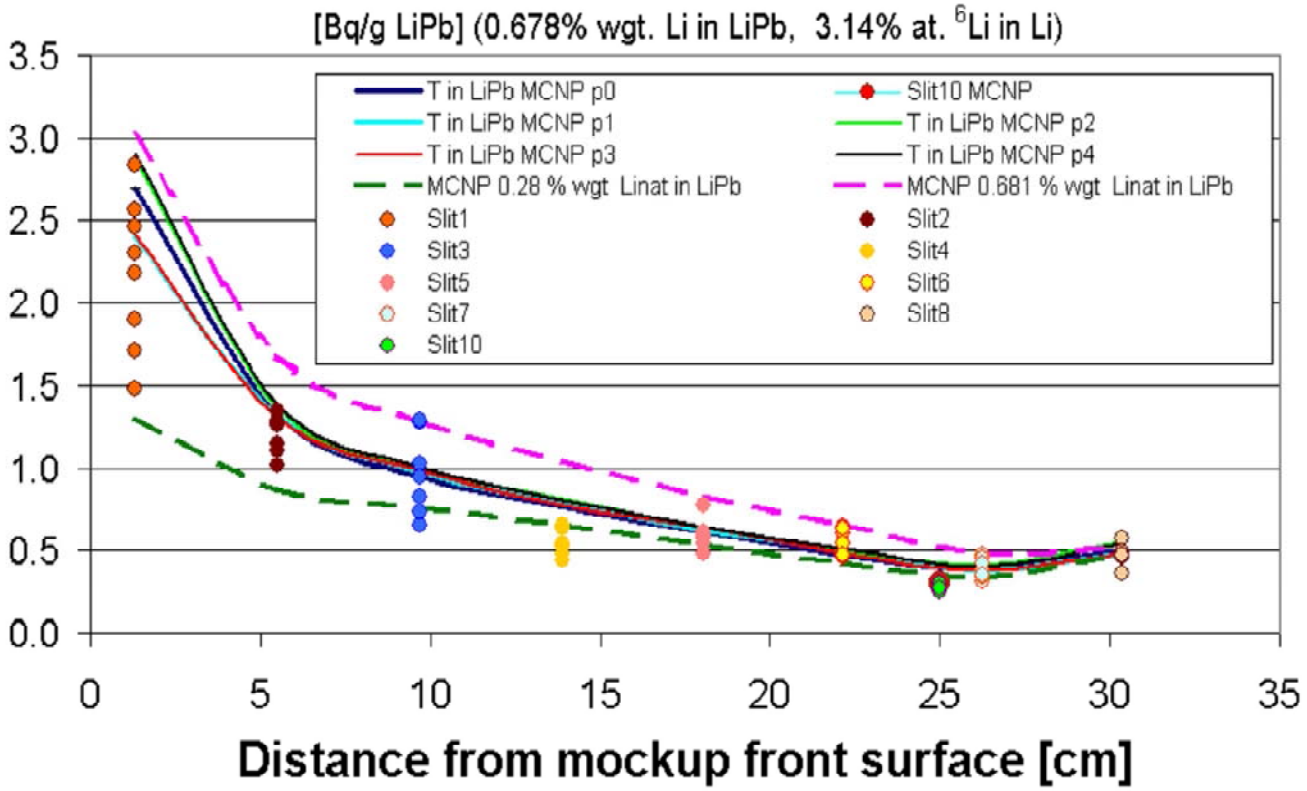
INTRODUCTION. The context of this work …

- **EFFDOC – 1113: "Measurements of tritium activity in HCLL TBM mock-up LiPb material irradiated in the Frascati experiment" (by W. W.Pohorecki) JEFF/EFF Meeting Paris, 31 May-2 June 2010**

- **T activity in LiPb mock-up material irradiated in Frascati: measurement and MCNP results.**

Figure 1: Slit 1-8, ^{3}H activity in LiPb



INTRODUCTION. The context of this work …

- **EFFDOC – 1135: "Analysis of the HCLL Blanket Mock-up Experiment" (by R. Villari et al.) JEFF/EFF Meeting Paris, [This meeting]**

Uncertainties on TPR determination

- Proposed definitive uncertainty on C/E comparison

✓ experimental errors (Li-6)	3.7%
✓ uncertainty on FNG source intensity	3%
✓ Monte Carlo calculation statistics	< 1%
✓ cross sections	< 2%
✓ Pb-Li composition	1%*

$$\Delta (C/E) \sim 5.3\ \% \quad (1\sigma)$$

- As a general result C/E are close to one within the total combined uncertainties (~±10% at 2σ level)

**Sensitivity of TPR to Li6 content : -0.5%/%*

Error propagation techniques for activation

Goal: "to analyse how ND uncertainty is transmitted to N"

$$\frac{d}{dt}N = AN \qquad N = (N_1, N_2, \ldots) \qquad \sigma = (\sigma_1, \sigma_2, \ldots) \qquad \Rightarrow \qquad N_i = N_i(\sigma)$$

1) Sensitivity / Uncertainty Analysis (S/U)

- Method based on the first order Taylor series to estimate uncertainty indices for each reaction cross section in a continuous irradiation scenario **(*linear approximation*)**

2) Monte Carlo Uncertainty Analysis (MC)

- To treat the global effect of all cross sections uncertainties in activation calculations, we have proposed an uncertainty analysis methodology based on Monte Carlo random sampling of the cross sections

- Assignment of a Probability Density Function (PDF) to each cross section

1. Sensitivity/Uncertainty Analysis

We assume:

$$N_i = N_i(\sigma, \lambda, \text{fission yields}, \phi(E), N_0) \Rightarrow N_i(\sigma) \approx N_i(\sigma_0) + \sum_{j=1}^{m} \left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\sigma_0} (\sigma_j - \sigma_{j0})$$

$$\frac{N_i(\sigma) - N_i(\sigma_0)}{N_i(\sigma_0)} \approx \sum_{j=1}^{m} \frac{\sigma_{j0}}{N_i(\sigma_0)} \left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\sigma_0} \frac{(\sigma_j - \sigma_{j0})}{\sigma_{j0}}$$

e_i — Relative error in N_i due to changes in cross-sections

ρ_{ij} — Cross-section sensitivity coefficient (FSAP, ASAP, …)

ε_j — Relative error in cross-sections

$$e_i = \rho_{i1}\varepsilon_1 + \rho_{i2}\varepsilon_2 + \cdots + \rho_{im}\varepsilon_m$$

$$Var[e_i] = \rho_{i1}^2\Delta_1^2 + \rho_{i2}^2\Delta_2^2 + \cdots + \rho_{im}^2\Delta_m^2$$

$$Var[e_i] = \rho_i^T V \rho_i$$

$$\rho_i = (\rho_{i1}, \quad \rho_{i2}, \quad \cdots \quad \rho_{im})$$

(sandwich formula)

$$Var(\varepsilon) = V$$

Information obtained processing ND

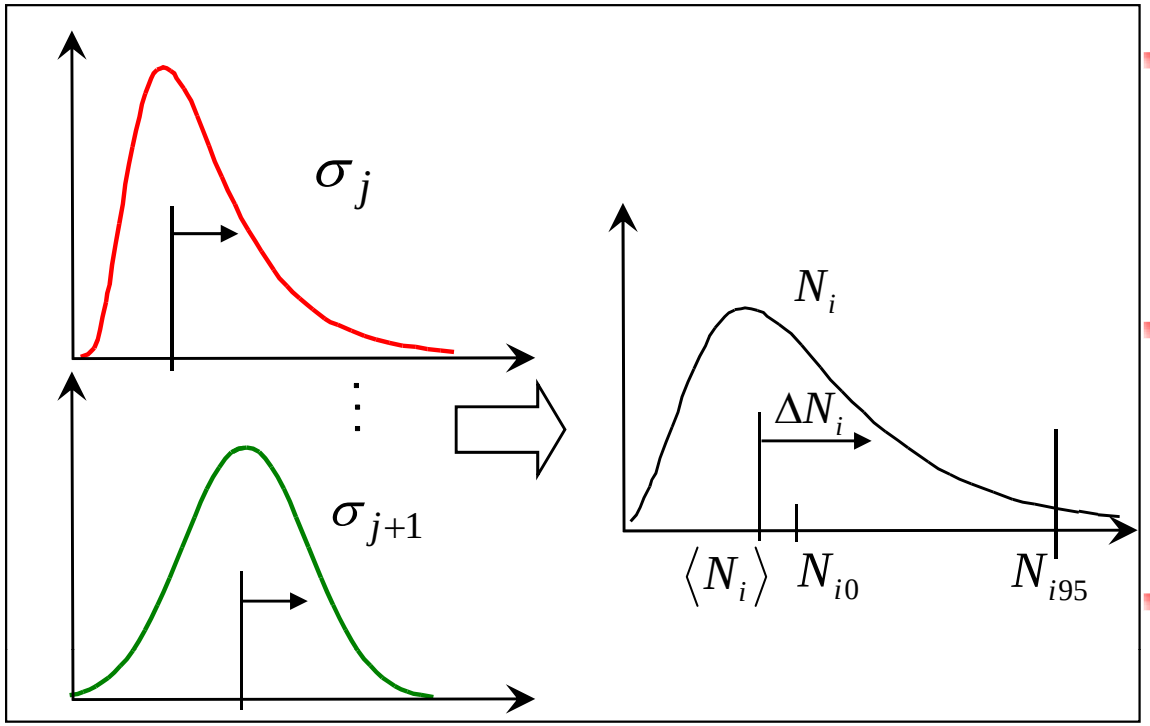
2. Monte Carlo method

- We use simultaneous random sampling of all the XS PDFs involved in the problem. PDF is assigned to each σ_j: $\sigma_j \rightarrow N(\sigma_{j0}, \mathrm{var}(\sigma_j)) \Rightarrow \varepsilon_j \rightarrow N(0, \Delta_j^2)$

$$\Rightarrow \text{For large values of } \Delta_j, \sigma_j \text{ could be negative!}$$

$$\log\begin{pmatrix} (\sigma_1/\sigma_{10}) \\ (\sigma_2/\sigma_{20}) \\ \vdots \\ (\sigma_m/\sigma_{m0}) \end{pmatrix} \rightarrow N(0,V)$$

- PDF assumed to be lognormal: $\log(\sigma_j/\sigma_{j0}) = \log(1+\varepsilon_j) \approx \varepsilon_j \rightarrow N(0, \Delta_j^2)$



- From the sample of the random vector σ, $\sigma = (\sigma_1 ..., \sigma_j ..., \sigma_m)$ the matrix **A** is computed and the vector of nuclide quantities $\boldsymbol{X}$ is obtained $N = (N_1 ..., N_i ..., N_n)$
- Repeating the sequence, we obtain a sample of isotopic concentration vectors. The statistic estimators of the sample can be estimated
- Enables to investigate the global effect of the complete set of $\Delta\sigma$ on N

A preliminary calculation …: ACAB2008/EAF2007

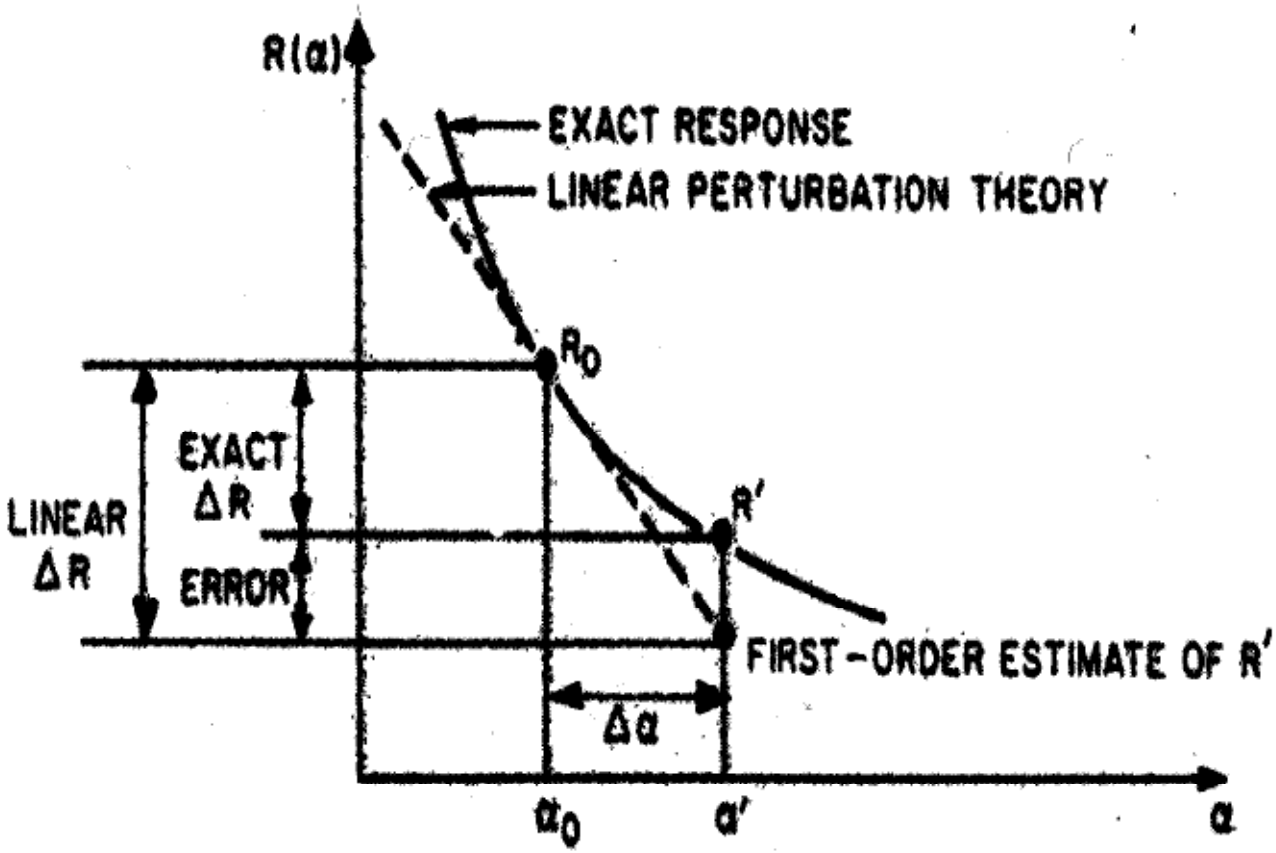
Figure 2: Tritium Uncertainty Prediction in SL1 and SL7 using EAF2007/UN

	SL1		SL7	
	Natural Abundance 7.25% Li6 in Li	Depleted Li6 3.14% Li6 in Li	Natural Abundance 7.25% Li6 in Li	Depleted Li6 3.14% Li6 in Li
Total Bq (at shutdown)	3.92	3.47	0.64	0.28
Only due to Li	3.78	3.33	0.64	0.28
Only Li6	0.96	0.40	0.62	0.26
Only Li7	2.82	2.93	0.02	0.02
Sensitivity Coefficiente: ρ = (DN/N) / (DXS/XS) in %				
Li6(n,T)He4	0.25	0.12	0.96	0.91
Li7(n,na)T	0.72	0.84	0.04	0.09
F19(n,T)		0.04		
Mg25(n,T)		1.14E-06		
…	…			
F19(n,nT)		6.36E-03		
Sensitivity/Uncertainty (%) = ρ*Δ				
Li6(n,T)He4	0.82	0.38	3.21	3.03
Li7(n,na)T	47.83	56.21	2.43	5.76
F19(n,T)		0.70		
…				
F19(n,nT)		0.85		
Sensitivity/Uncertainty (%)= (ρ*Δ)	**47.84**	**56.22**	**4.03**	**6.51**
Uncertainty with Monte Carlo				
Mean value	4.67	4.27	0.65	0.29
Relative error (%)	**58.62**	**67.03**	**4.78**	**8.77**

- ρ : is the sensitivity coefficient for the tritium production
- Δ : is the corresponding relative error collapsed in 1 group
- the index "ρΔ" that can be used to rank cross sections inducing the highest uncertainties

To take into account …: Linear Perturbation Theory

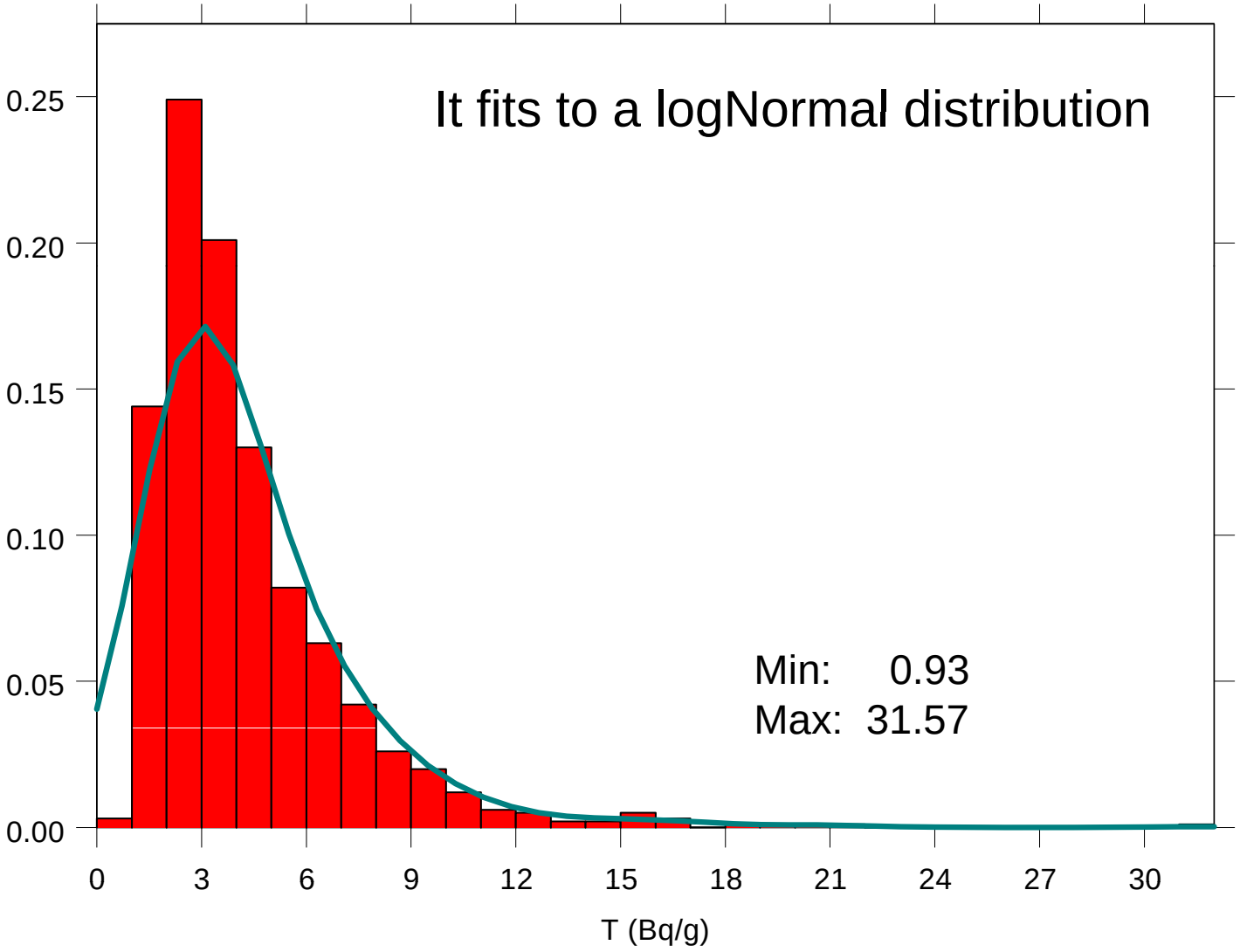
Applicability of 1st Taylor-series expansion



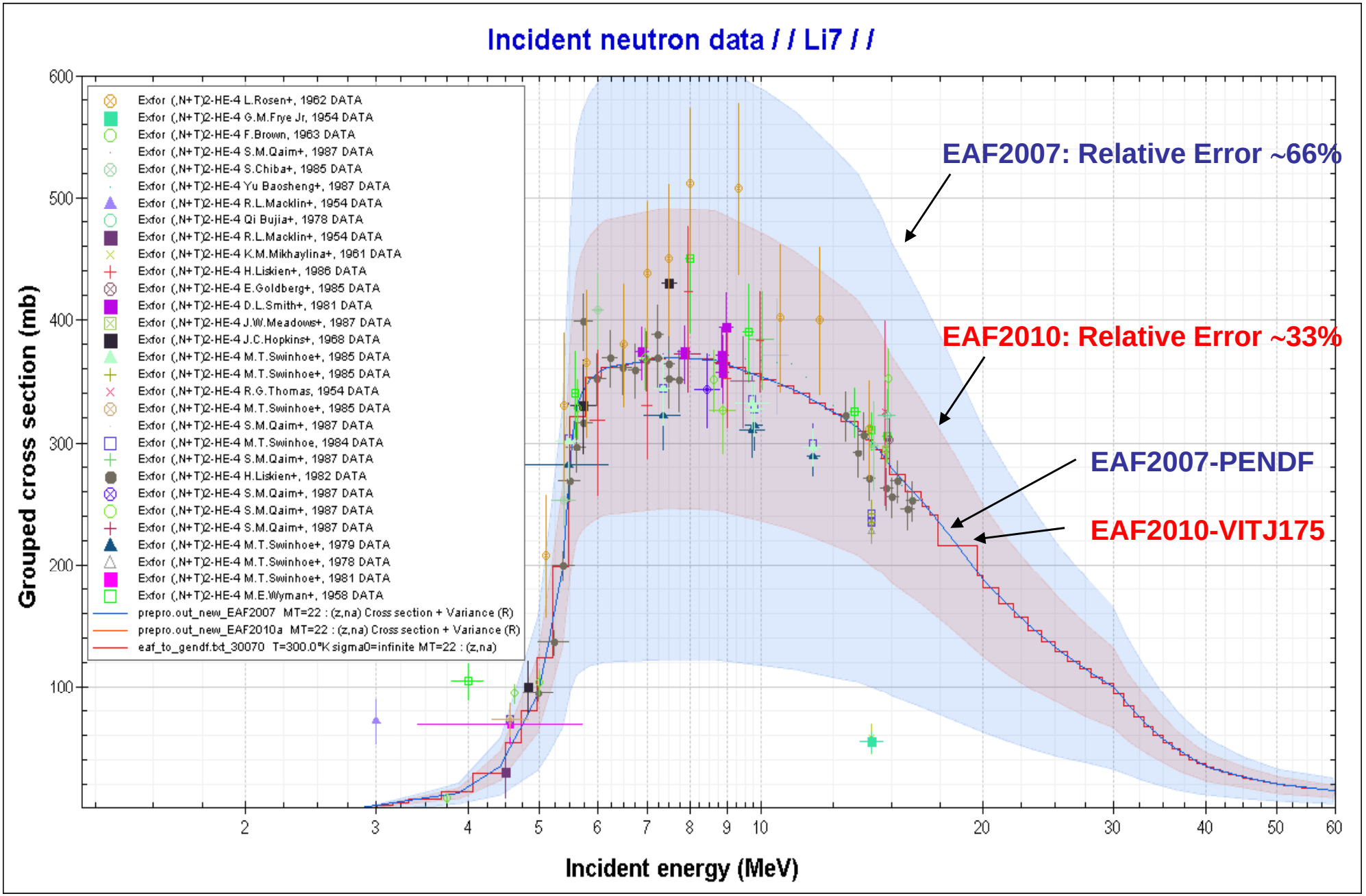
The deterministic approach should be used wherever it provides sufficiently accurate results. Normally, this will be the case when errors are relatively small and the conditions not extreme.

To take into account …: Monte Carlo sampling

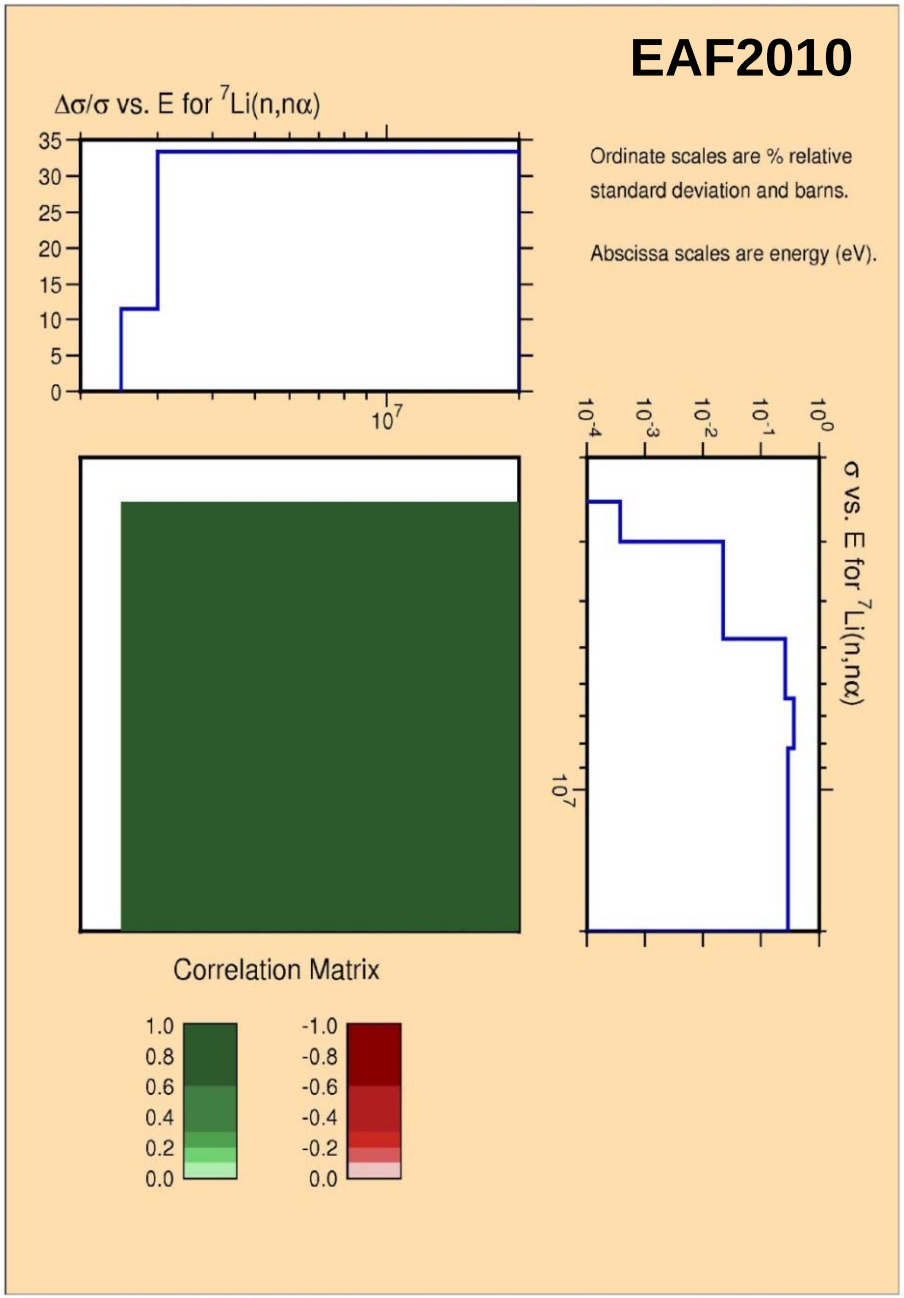
Mean Value: T_M= 4.27 Bq/g; and relative error : 67.03%



^{7}Li(n,T) – EAF 2010&2007 Uncertainties



^{7}Li(n,T) – EAF 2010&2007: Covariance matrix



- Given ***V*** the G-by-G variance matrix of the relative XSs vector, the variance Δ^2 of the relative spectrum-averaged cross section is $\Delta^2 = \omega^T V \omega$

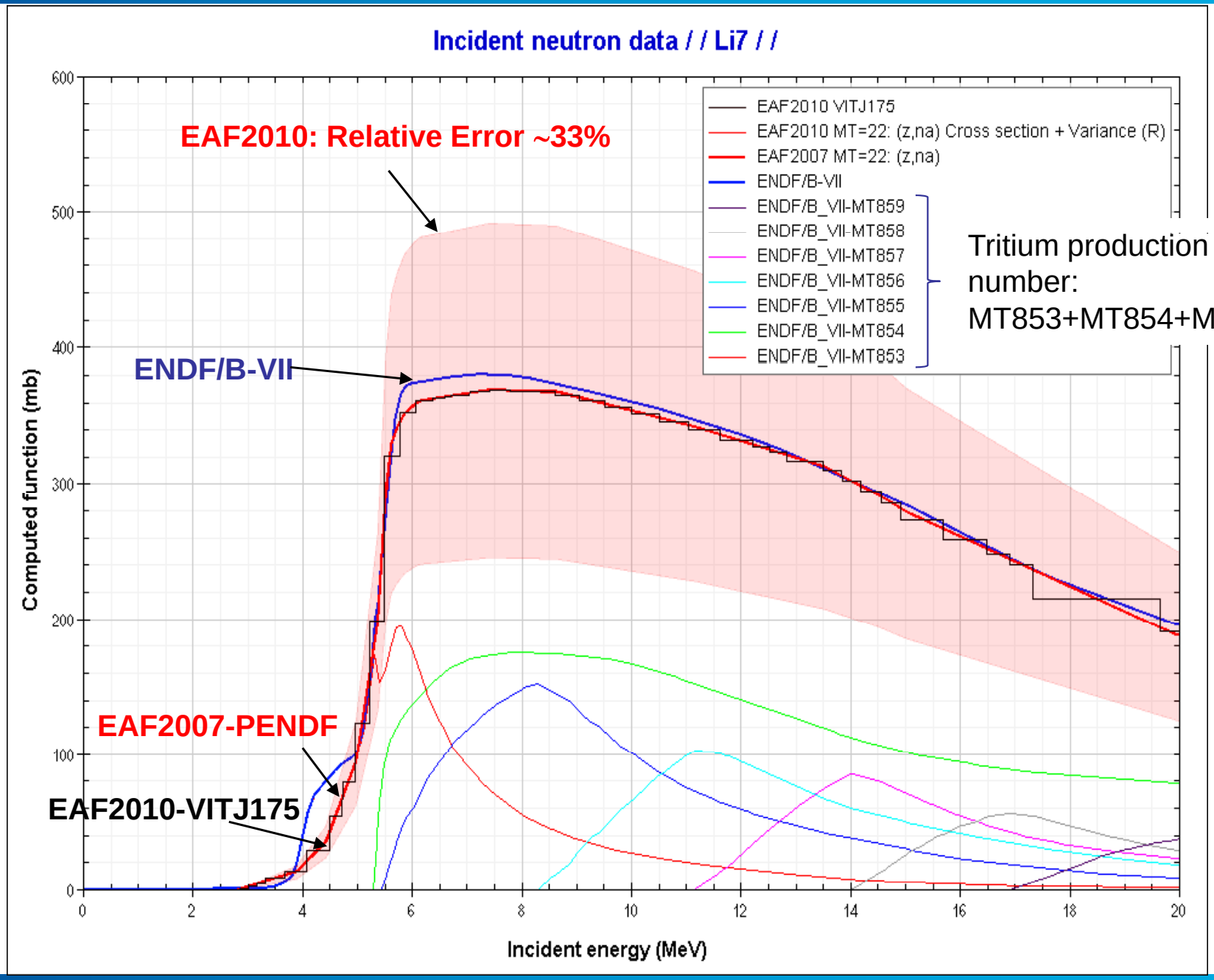
  ; with $\omega = [\frac{\phi_1}{\bar{\phi}}\frac{\sigma_1}{\sigma^{eff}}, \cdots, \frac{\phi_G}{\bar{\phi}}\frac{\sigma_G}{\sigma^{eff}}]^T$

- Assuming $\Delta^2_{I=1,EAF}$ (relative error, Δ)
  $\rightarrow \Delta_{I=1,EXP} = \Delta_{I=1,EAF}/3$

Uncert_1group (EAF2007) = Δ	$\Delta^2_{EAF2007}$	Relative Exp Error (%)
Li6(n,T)He4	0.01	3.33
Li7(n,na)T	4.00	66.67
F19(n,T)	0.36	20.00
…		
F19(n,nT)	16.00	133.33

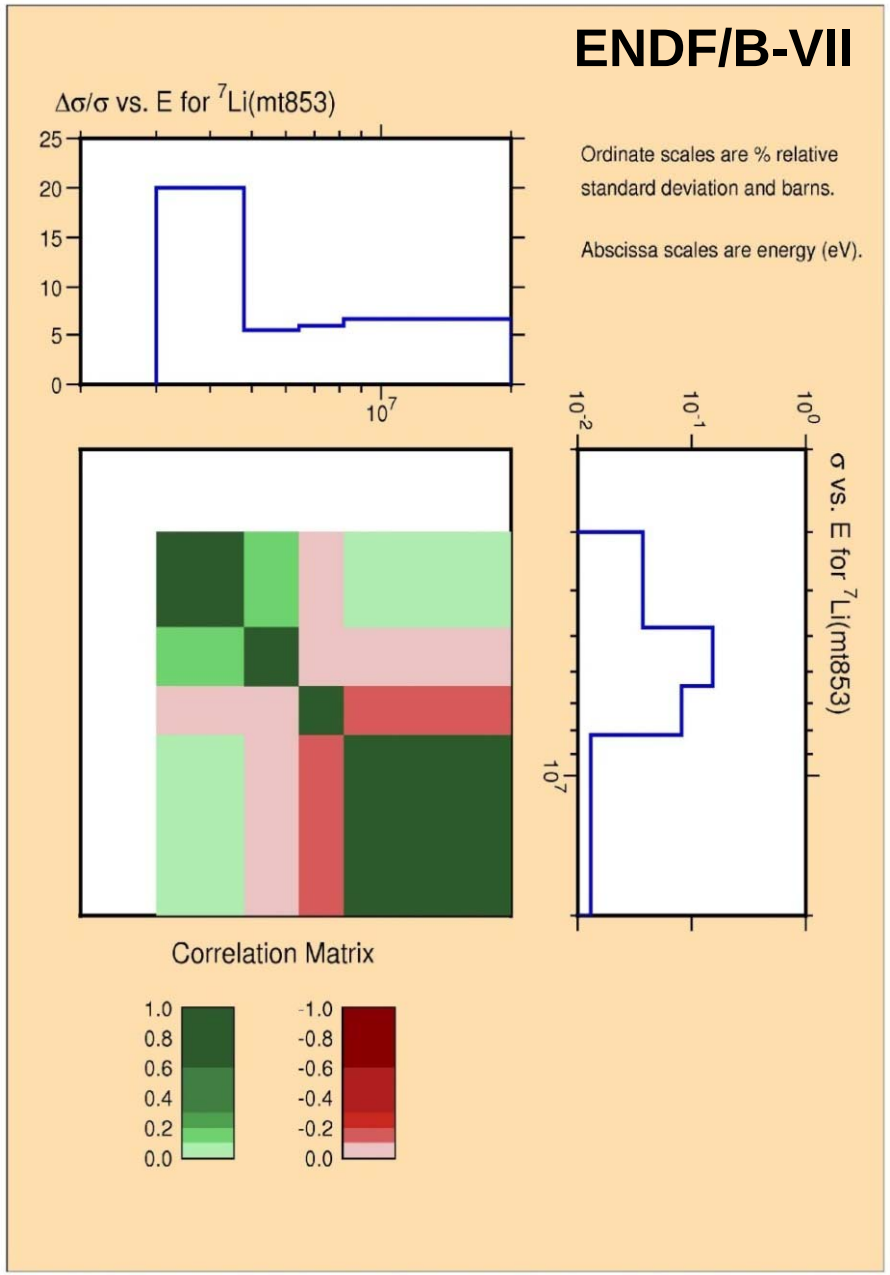
Uncert_1group (EAF2010) = Δ	$\Delta^2_{EAF2010}$	Relative Exp Error (%)
Li6(n,T)He4	0.01	3.33
Li7(n,na)T	1.00	33.33
F19(n,T)	0.36	20.00
…		
F19(n,nT)	4.00	66.67

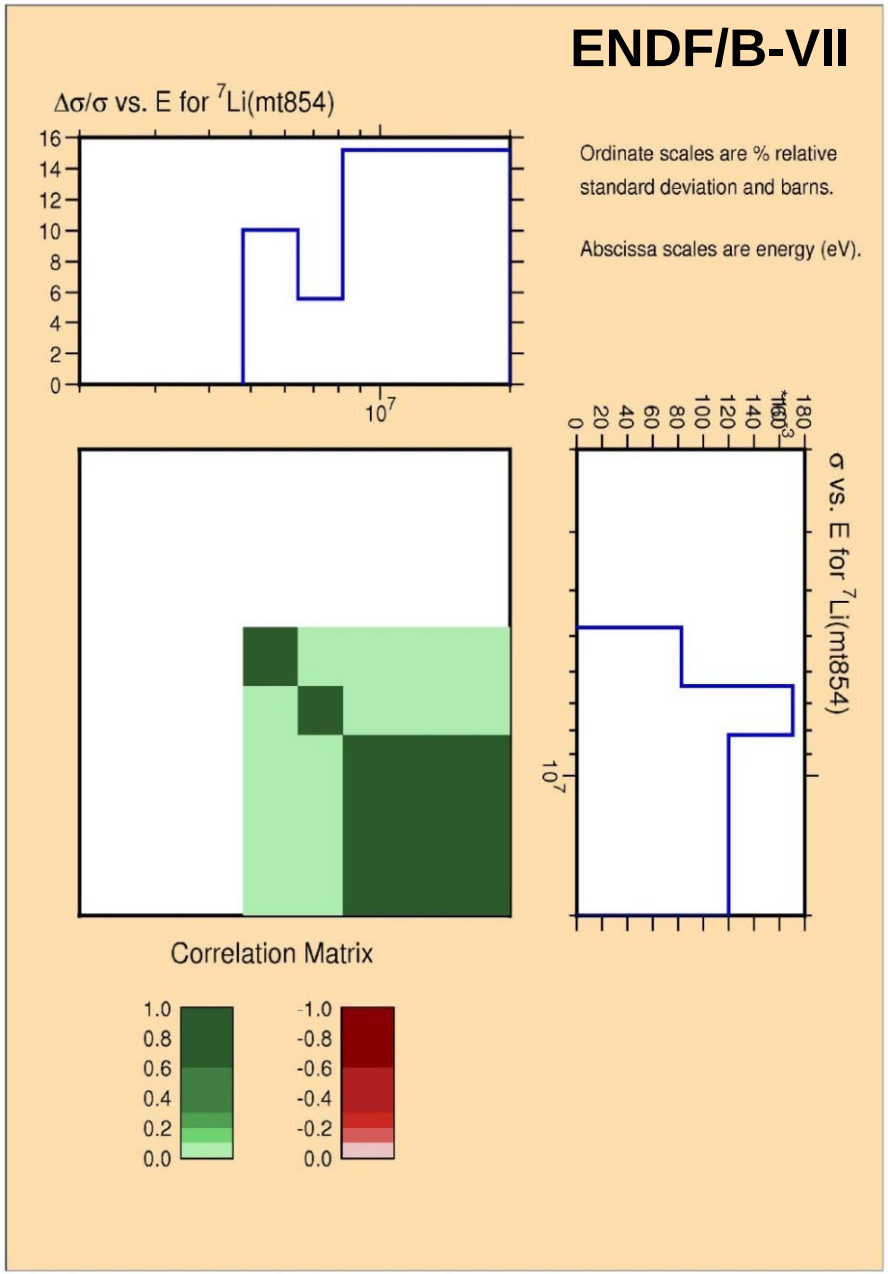
^{7}Li(n,T) - ENDF/B-VII vs EAF2010



Tritium production is not in one MT number:
MT853+MT854+MT855+ …=(n,n'at)

^{7}Li(n,T) - ENDF/B-VII: Covariance Matrix in 44g





^{7}Li (n,T) - ENDF/B-VII: in Δ_{1g} for SL1

Cross-sections collapsed in 1 group with SL1

	MT853	MT854	MT855	MT856	MT857	MT858	MT859
XS MTs_1g	7.12E-03	4.76E-02	1.48E-02	2.10E-02	2.71E-02	1.53E-02	2.19E-33
MTs/MTtotal	0.05	0.36	0.11	0.16	0.20	0.12	0.00

Relative cocariance matrix

	MT853	MT854	MT855	MT856	MT857	MT858	MT859
MT853	2.49E-03	0.00E+00	2.02E-04	-2.17E-06	-3.54E-05	-2.22E-05	-5.78E-20
MT854	0.00E+00	1.15E-03	-3.16E-04	-4.86E-04	-6.74E-04	-3.38E-04	-7.81E-18
MT855	2.02E-04	-3.16E-04	1.56E-03	1.70E-04	-1.42E-04	-7.21E-05	-5.10E-19
MT856	-2.17E-06	-4.86E-04	1.70E-04	2.07E-03	-2.60E-04	-1.25E-04	-1.36E-18
MT857	-3.54E-05	-6.74E-04	-1.42E-04	-2.60E-04	2.11E-03	2.24E-04	-2.97E-18
MT858	-2.22E-05	-3.38E-04	-7.21E-05	-1.25E-04	2.24E-04	3.16E-03	3.10E-17
MT859	-5.78E-20	-7.81E-18	-5.10E-19	-1.36E-18	-2.97E-18	3.10E-17	0.00E+00

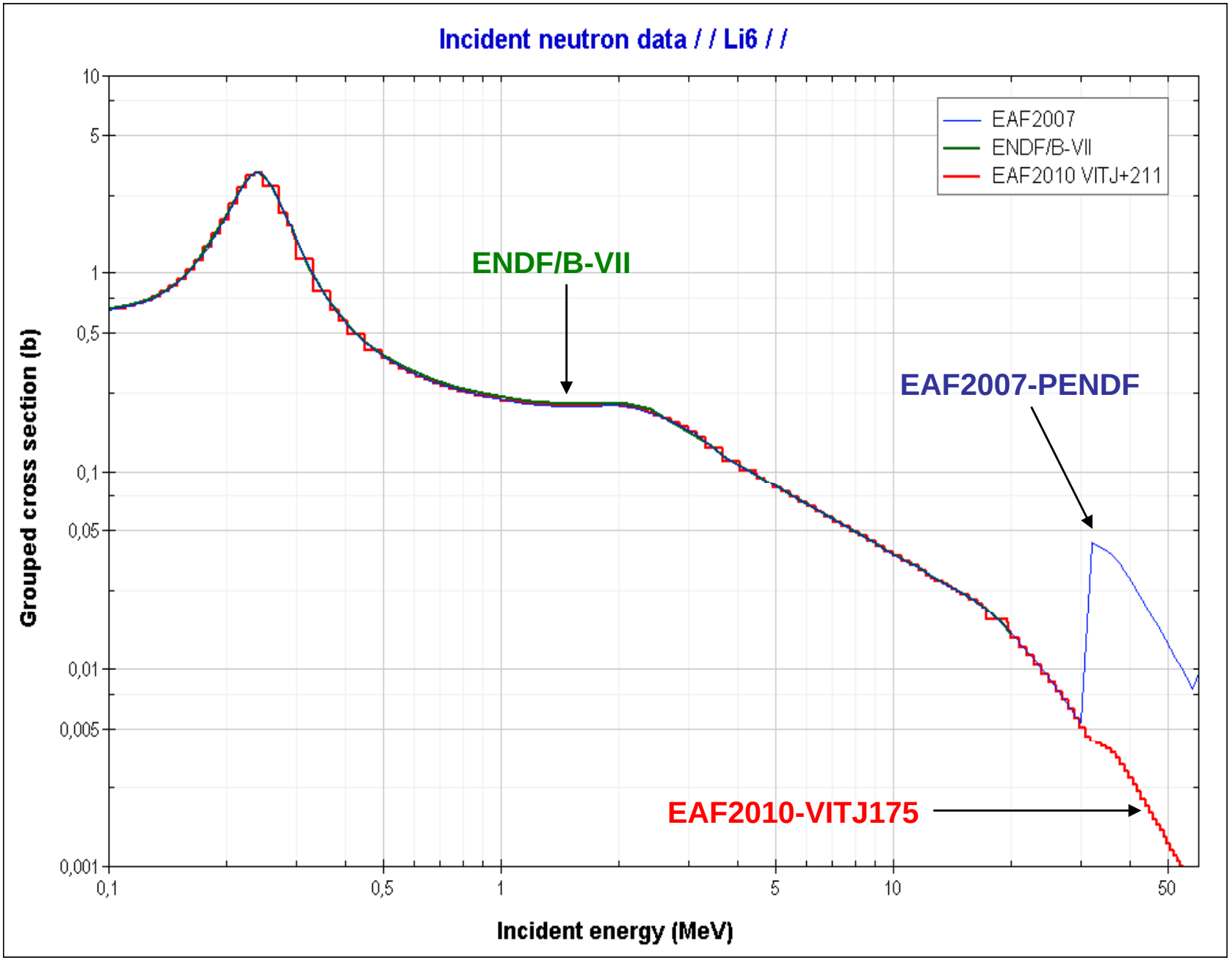
Relative error(%) covariance matrix

	MT853	MT854	MT855	MT856	MT857	MT858	MT859
MT853	4.99	0.00	1.42	0.15	0.59	0.47	0.00
MT854	0.00	3.39	1.78	2.20	2.60	1.84	0.00
MT855	1.42	1.78	3.95	1.31	1.19	0.85	0.00
MT856	0.15	2.20	1.31	4.55	1.61	1.12	0.00
MT857	0.59	2.60	1.19	1.61	4.59	1.50	0.00
MT858	0.47	1.84	0.85	1.12	1.50	5.62	0.00
MT859	0.00	0.00	0.00	0.00	0.00	0.00	0.00

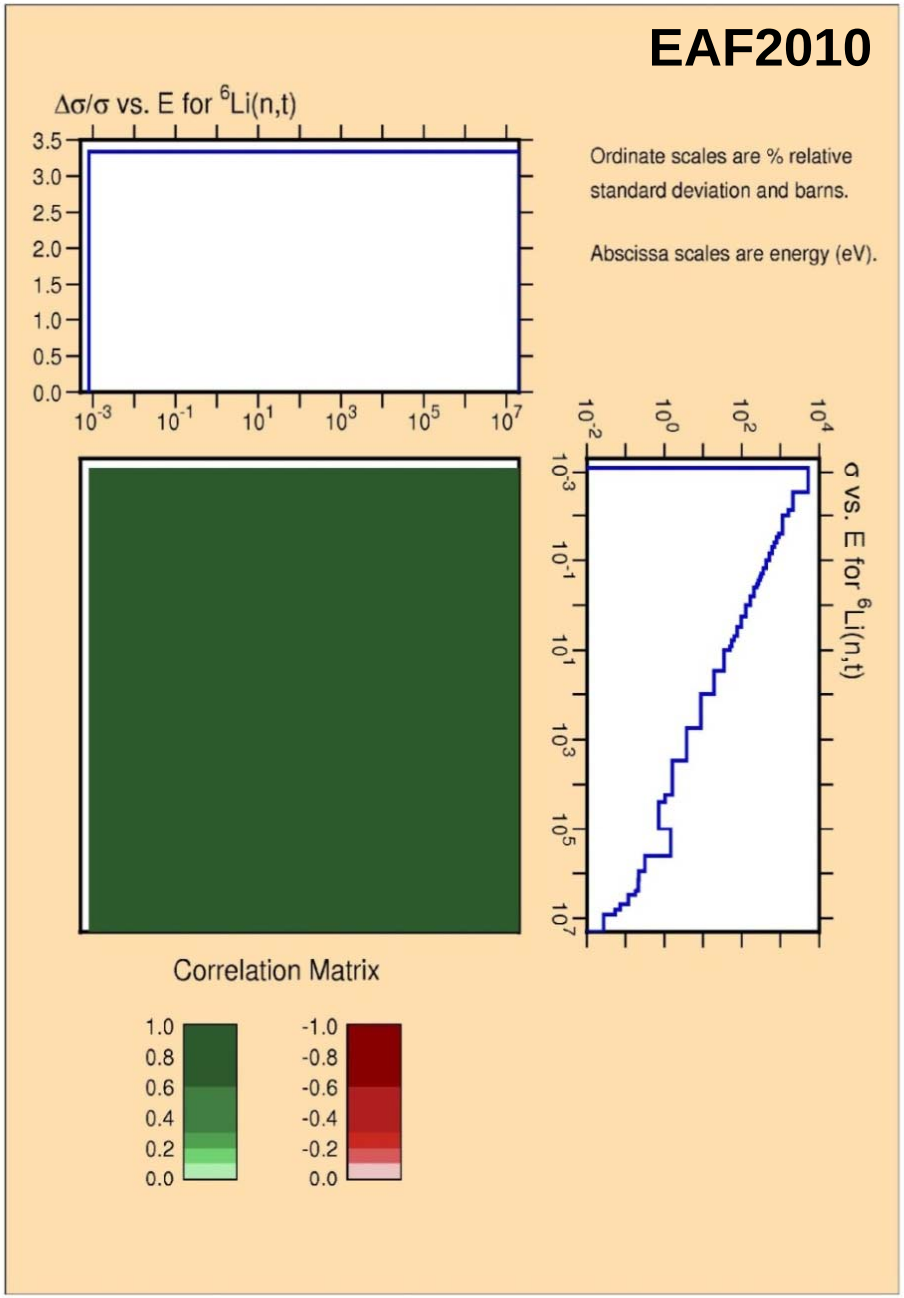
Rel. Err. in 1g (%)	1.17

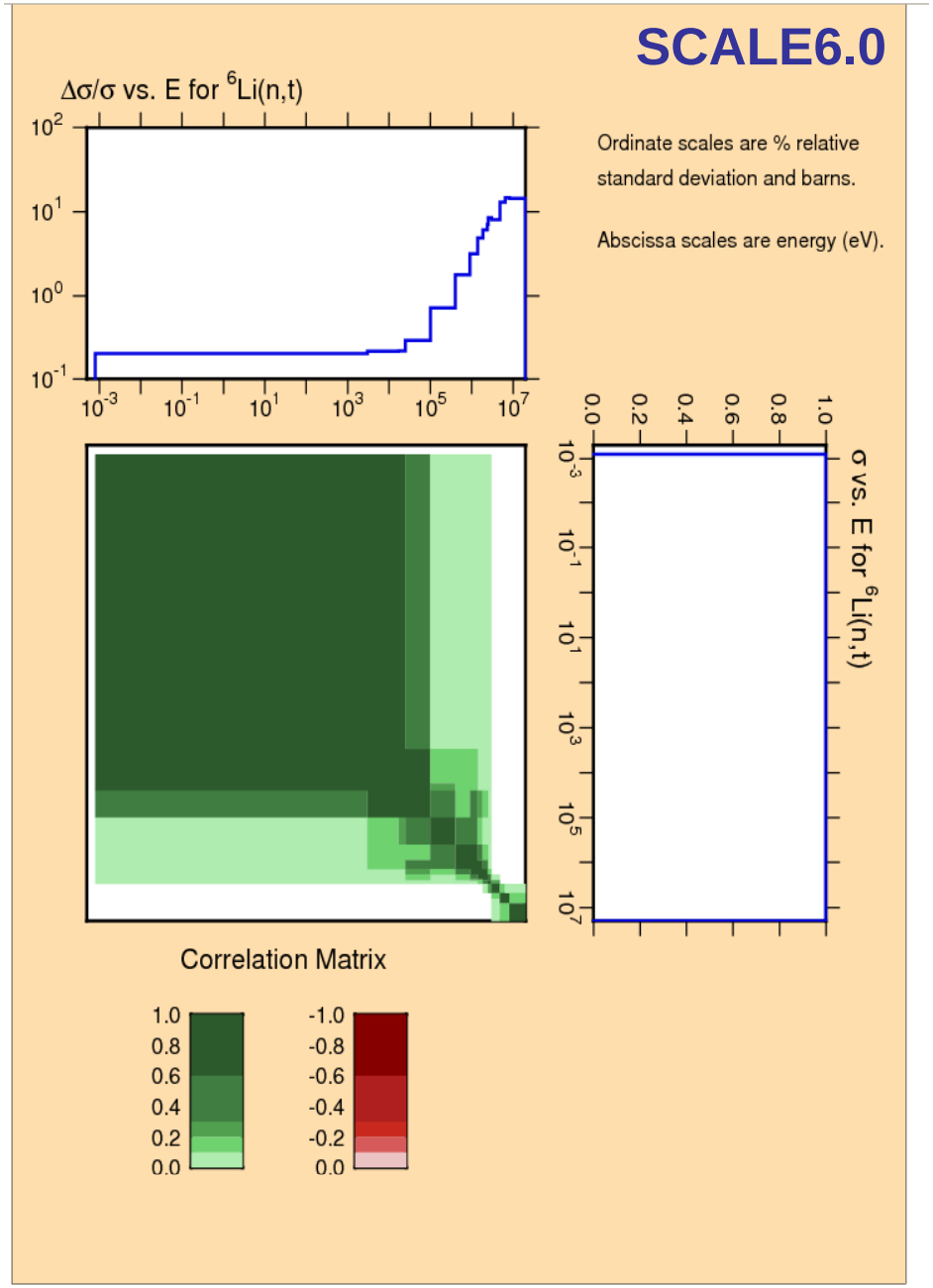
The relative error in 1group “lumped XS“ is only **1.17%** !!!

^{6}Li(n,T) - ENDF/B-VII vs EAF2010

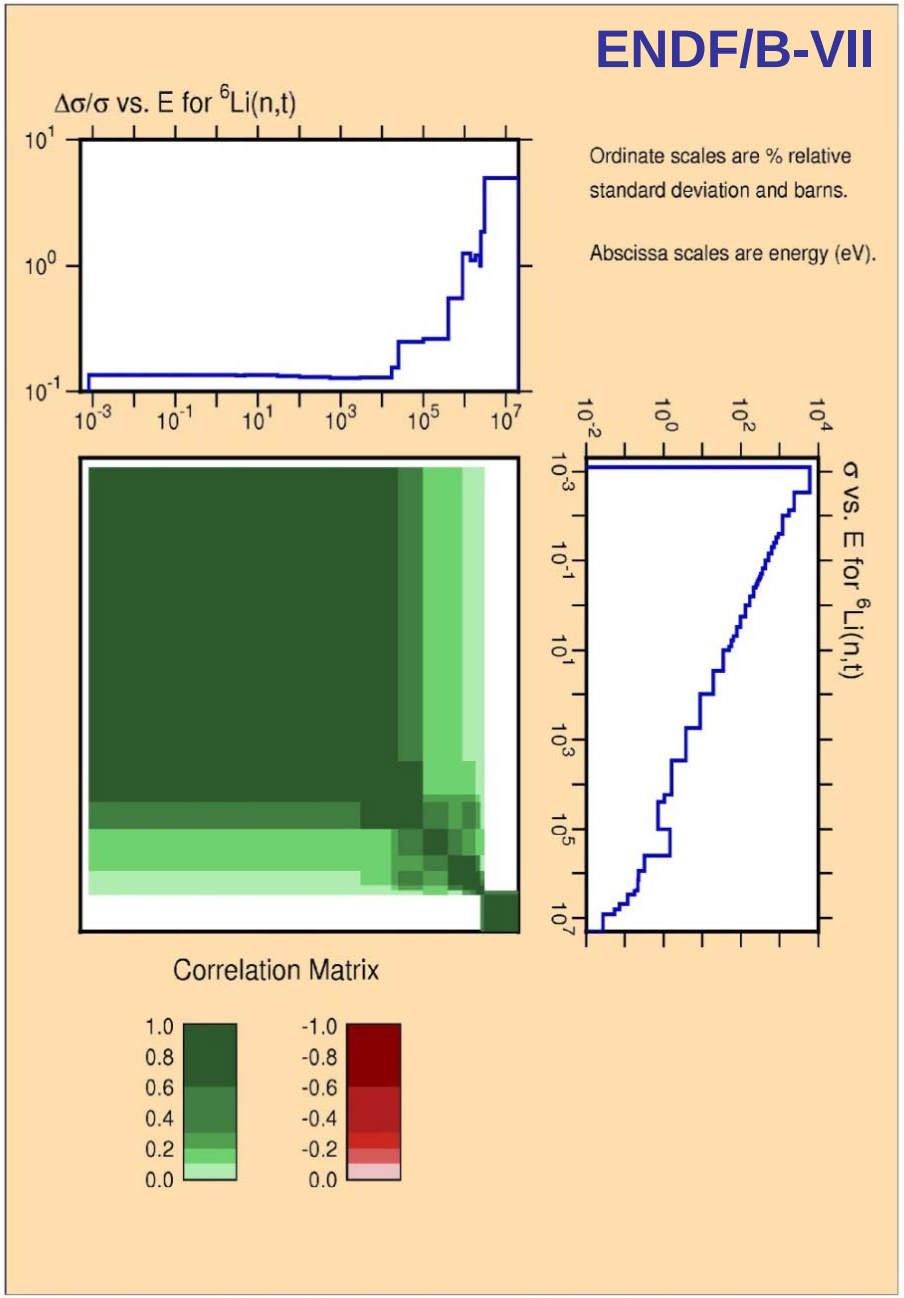


^{6}Li(n,T) – EAF 2010/2007 and SCALE6.0: Covariance matrix





^{6}Li(n,T) - ENDF/B-VII : Covariance Matrix in 44g



	SL1	
Uncert_1group (ENDF/B-VII) = Δ	$\Delta^2_{ENDF/B-VII}$	Relative Exp Error (%)
Li6(n,T)He4	6.64E-06	0.26

	SL7	
Uncert_1group (ENDF/B-VII) = Δ	$\Delta^2_{ENDF/B-VII}$	Relative Exp Error (%)
Li6(n,T)He4	1.59E-06	0.13

Processing TENDL2010: ^{7}Li(n,T) , ^{6}Li(n,T) and ^{240}Pu(n,γ)

Objective:

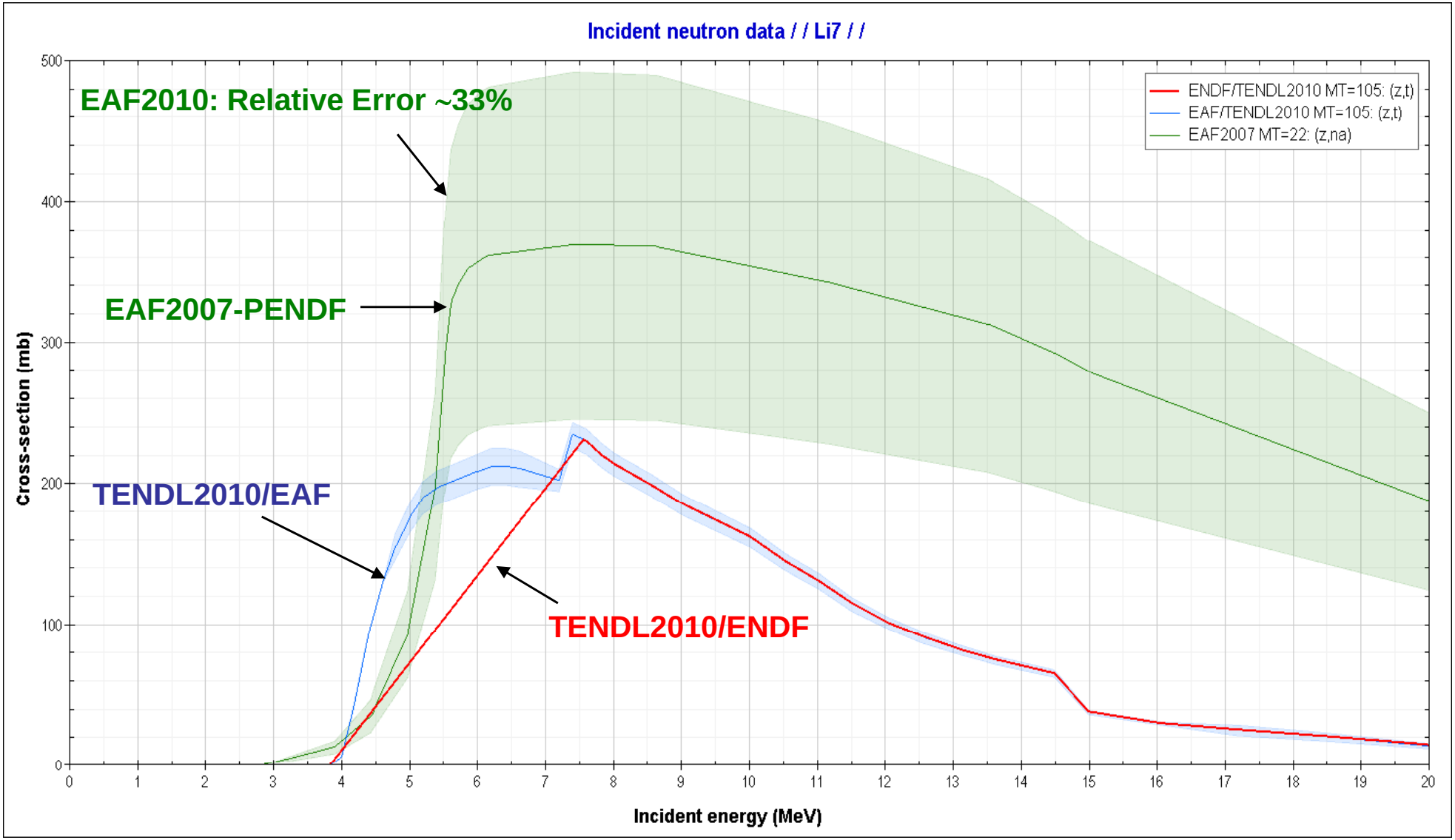
"Processing and testing **TENDL2010/EAF** and **TENDL2010/ENDF** to activation calculations"

- **Processing EAF/TENDL2010**

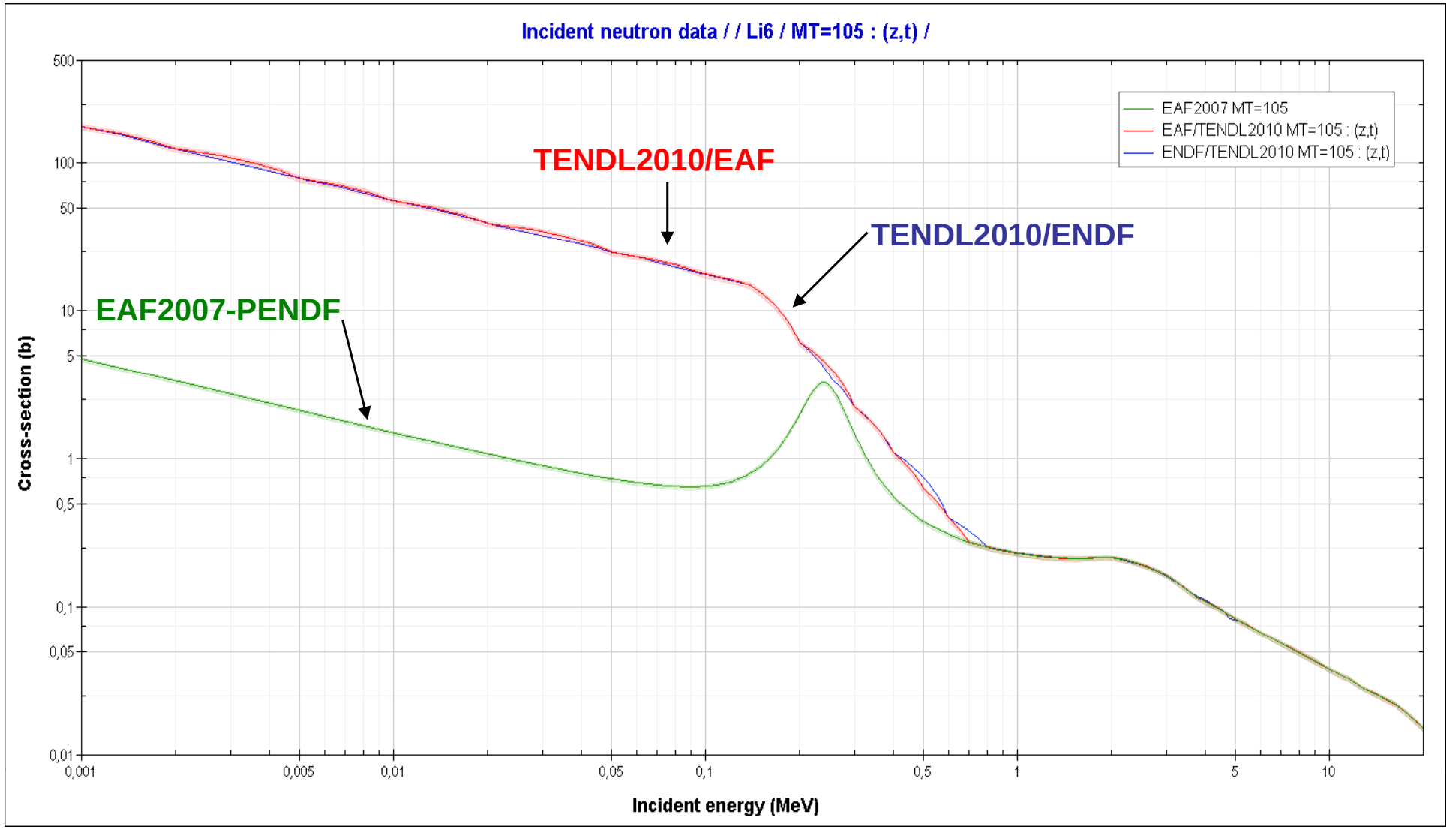
  -Problems:
  - MT=18 and MT=102 with more than 10000 energy points
  - Different channels in the variance and cross section files
  - No uncertainties for isomeric/branching reactions

- **Processing ENDF/TENDL2010**
  - Problem:
    - NJOY/ERRORR-URR for Pu240

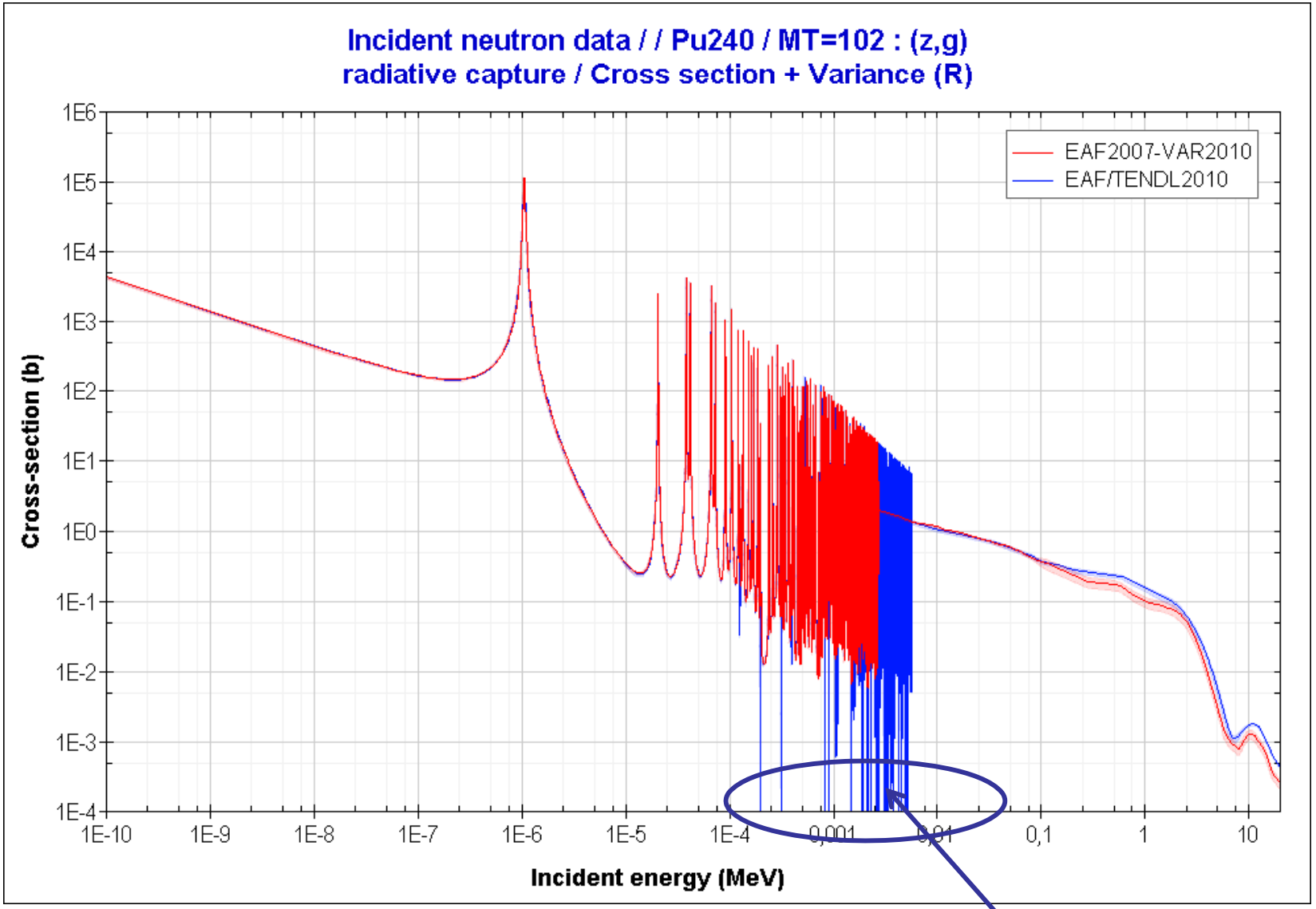
^{7}Li(n,T) – TENDL2010



^{6}Li(n,T) – TENDL2010

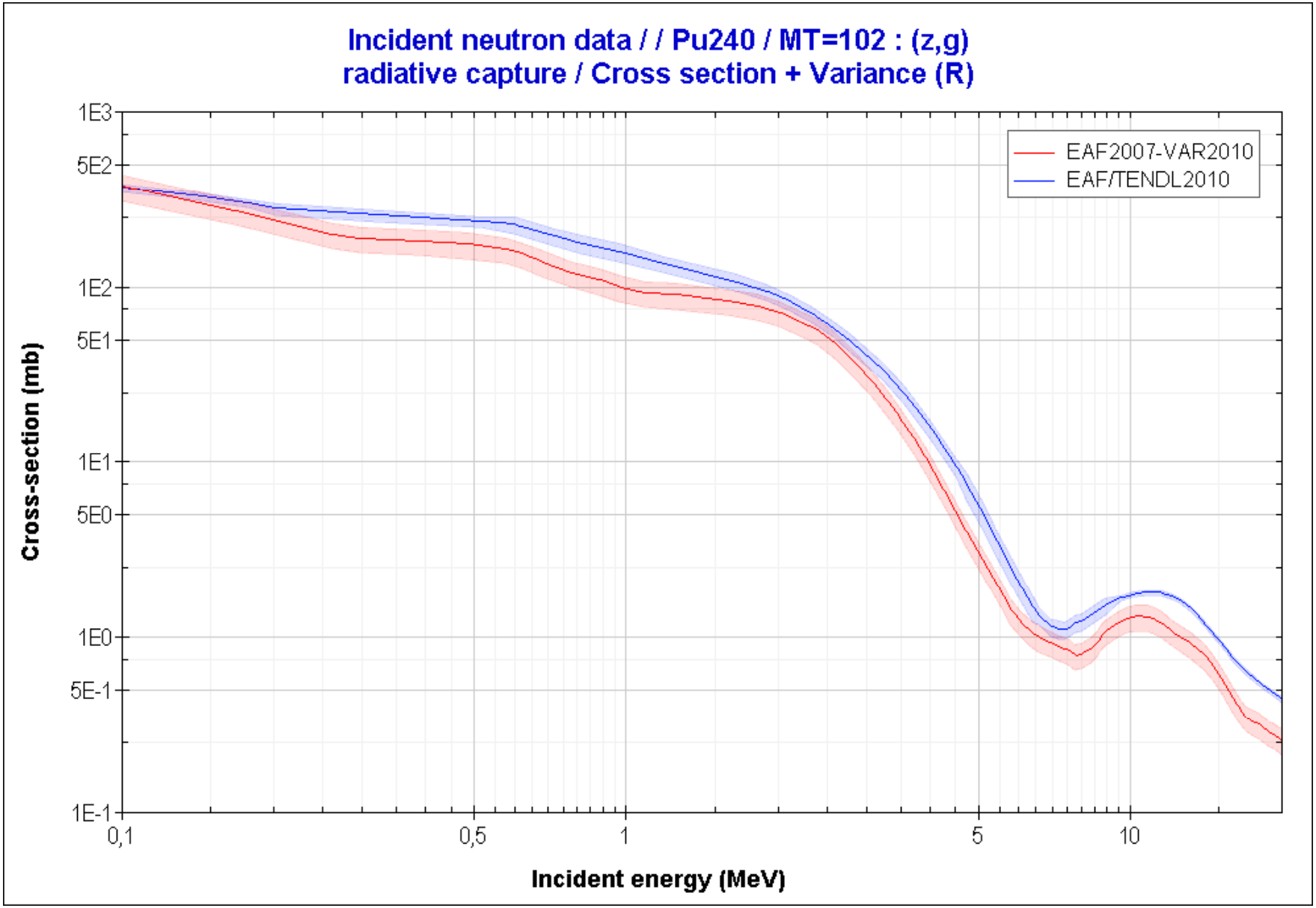


^{240}Pu(n,γ) – EAF2007 vs TENDL2010/EAF

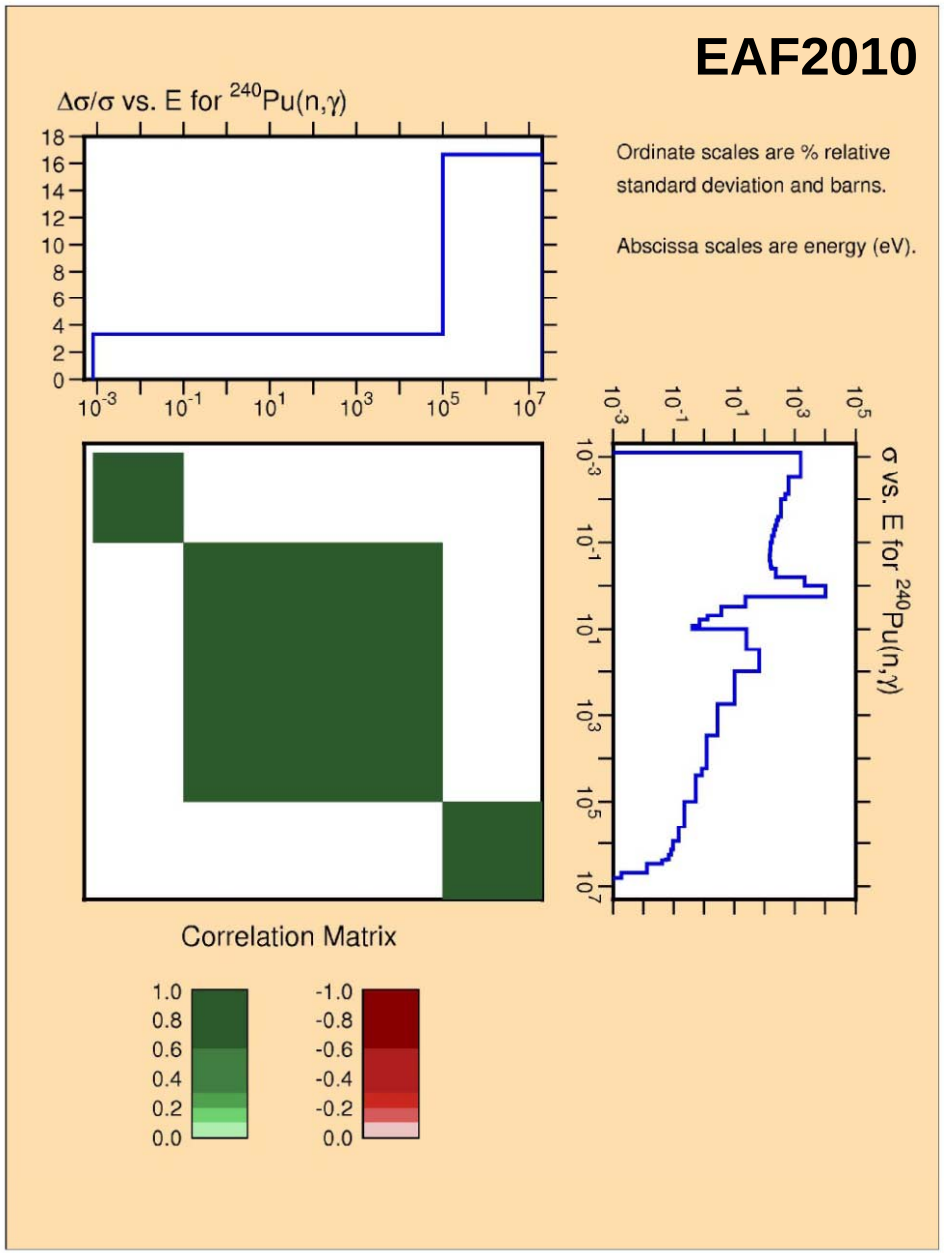


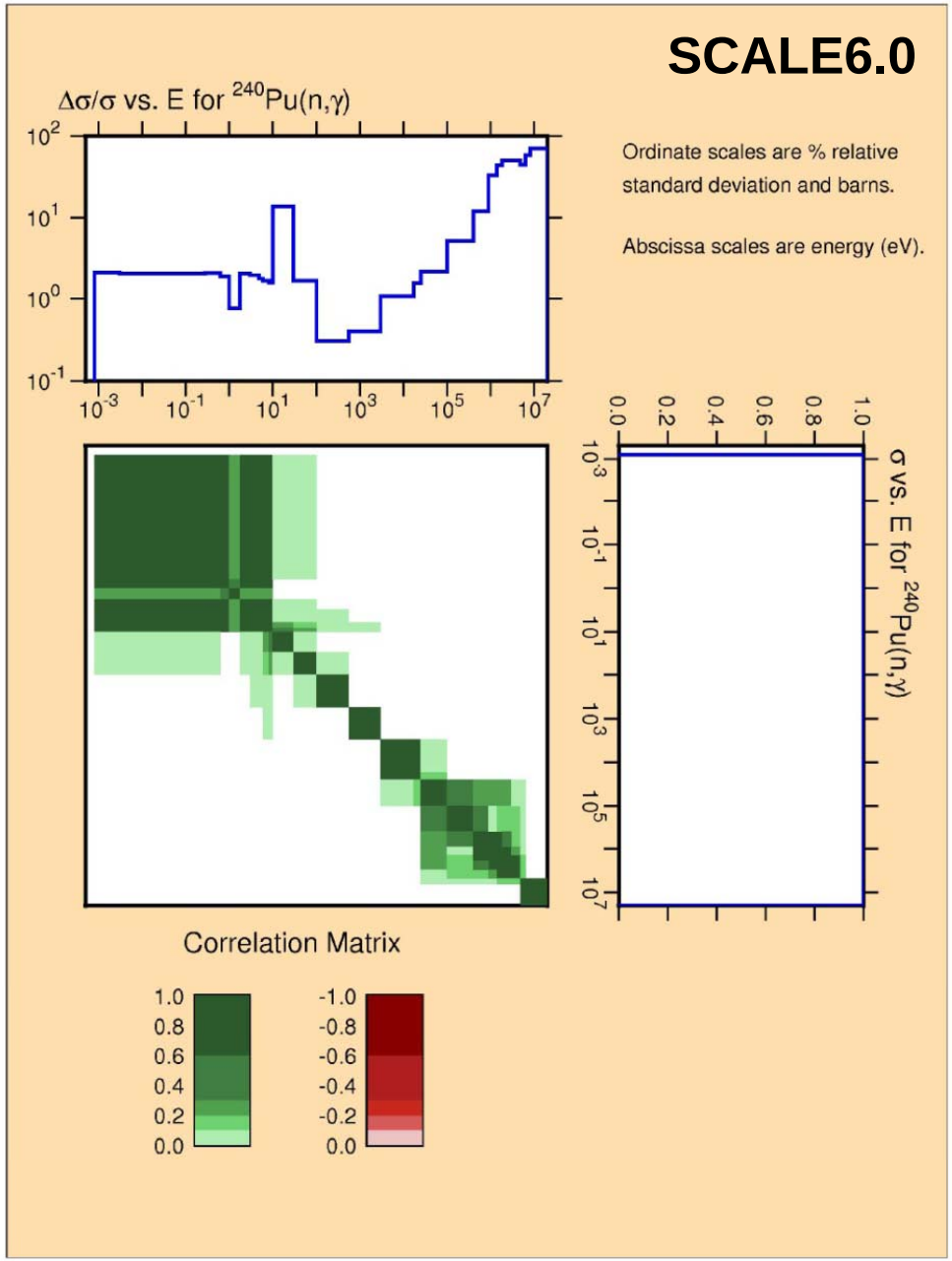
These are related to not-accurate-resonance widths

^{240}Pu(n,γ) – EAF2007 vs TENDL2010/EAF



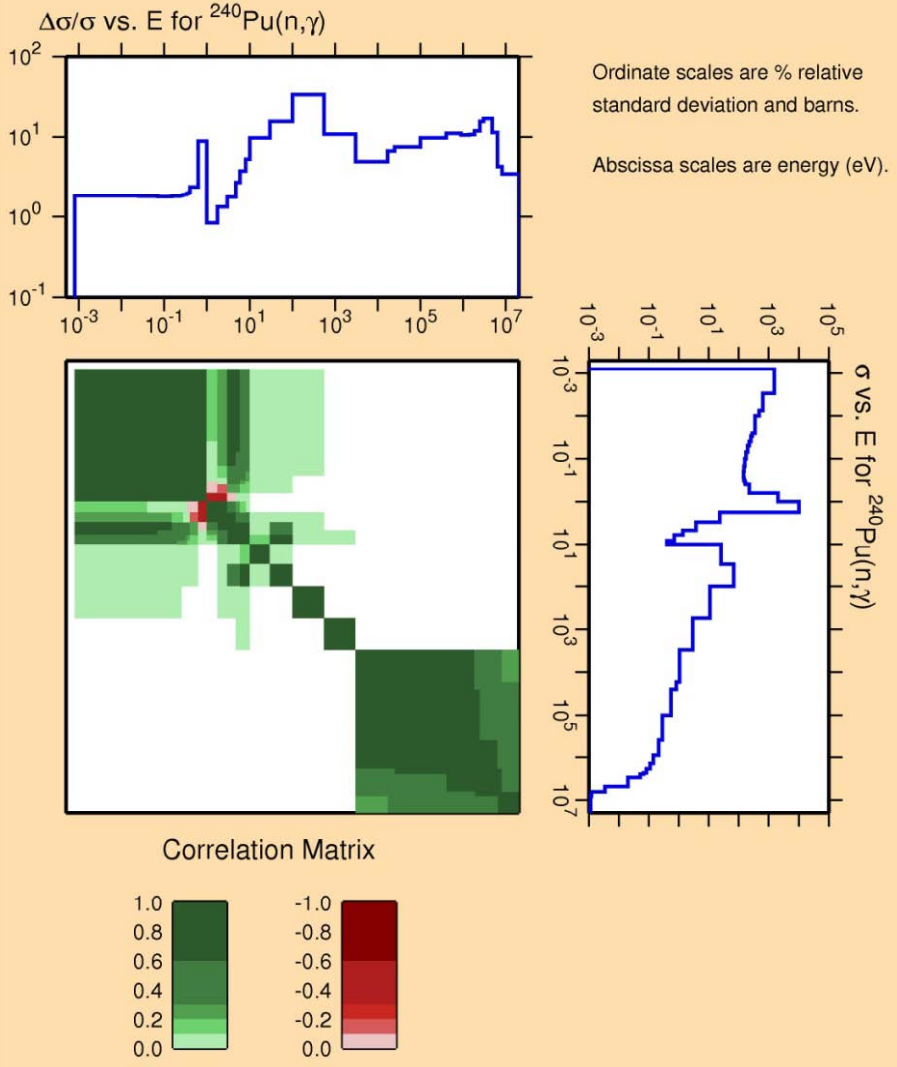
^{240}Pu(n,γ) Covariance Matrix in 44g





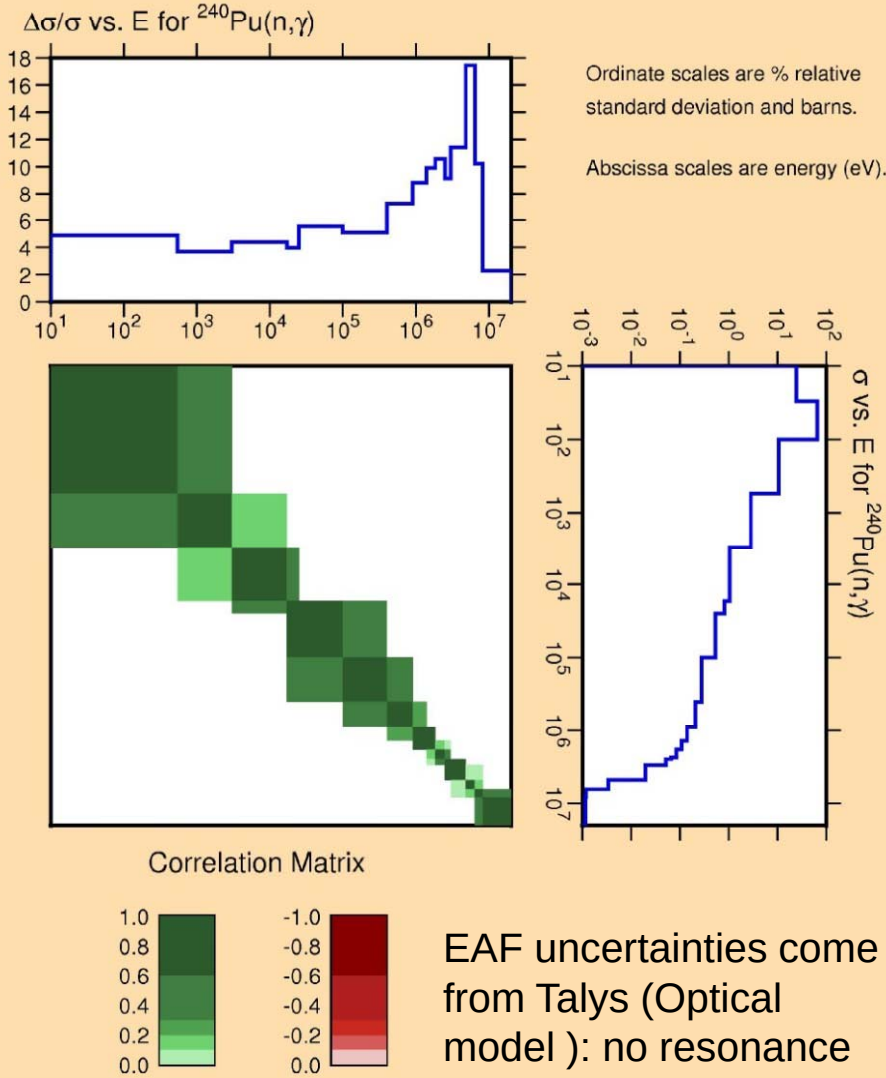
^{240}Pu(n,γ) Covariance Matrix in 44g

TENDL2010/ENDF



ENDF files (where MF32 and MF33 are used)

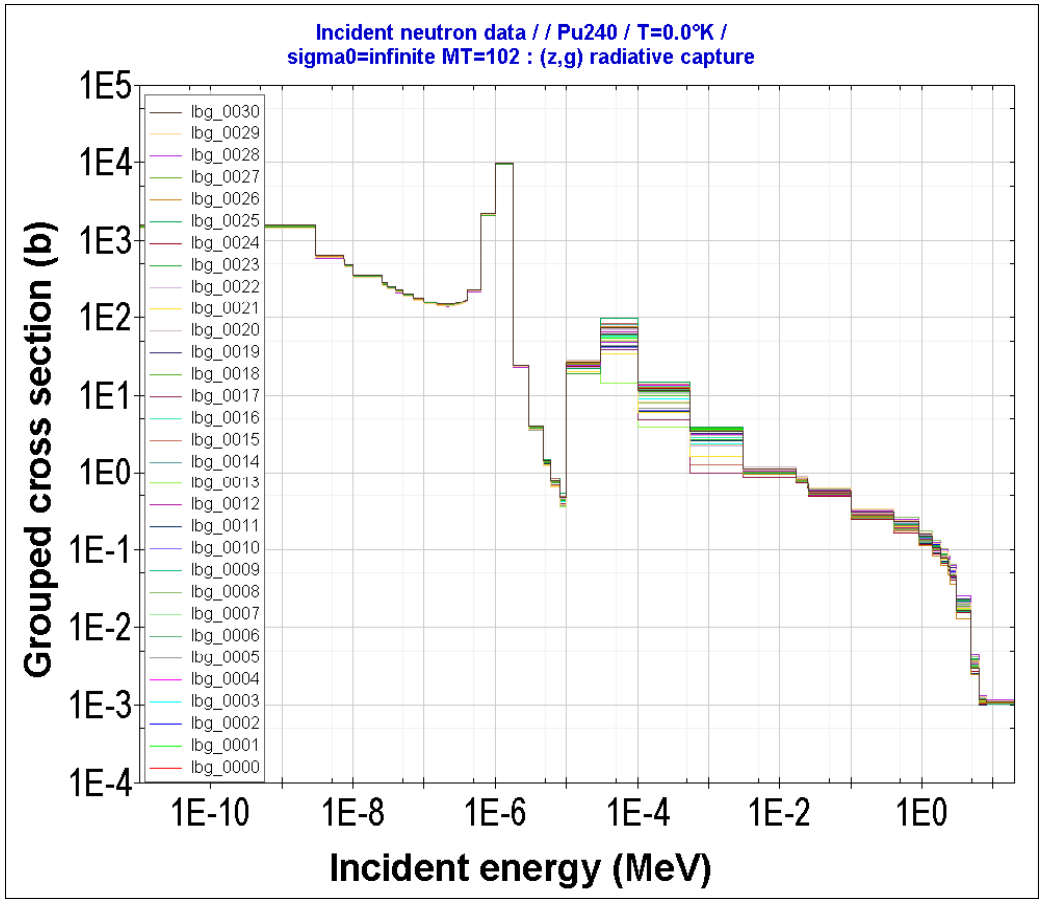
TENDL2010/EAF



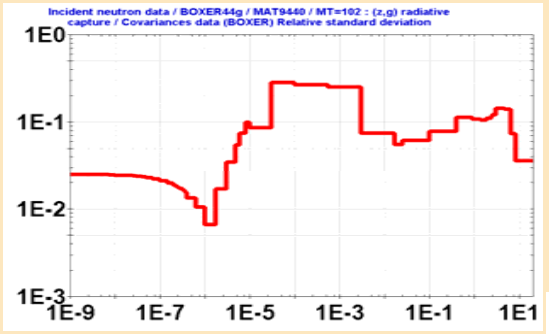
EAF uncertainties come from Talys (Optical model): no resonance info (no structure at low energy)

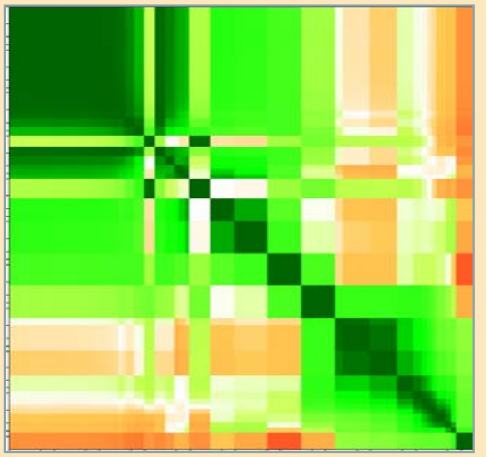
^{240}Pu(n,γ) Covariance Matrix in 44g from RANDOM/EAF

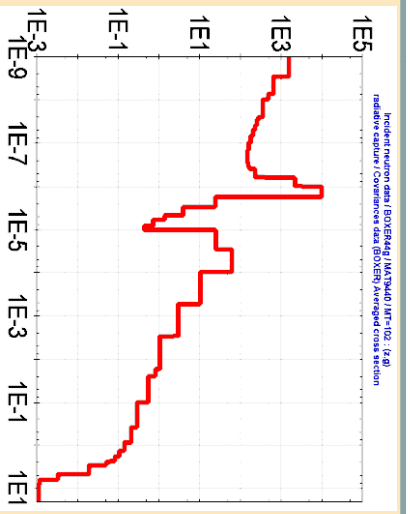
How can we calculate the correlation matrix based on the random files?



TENDL2010/RANDOM EAF files

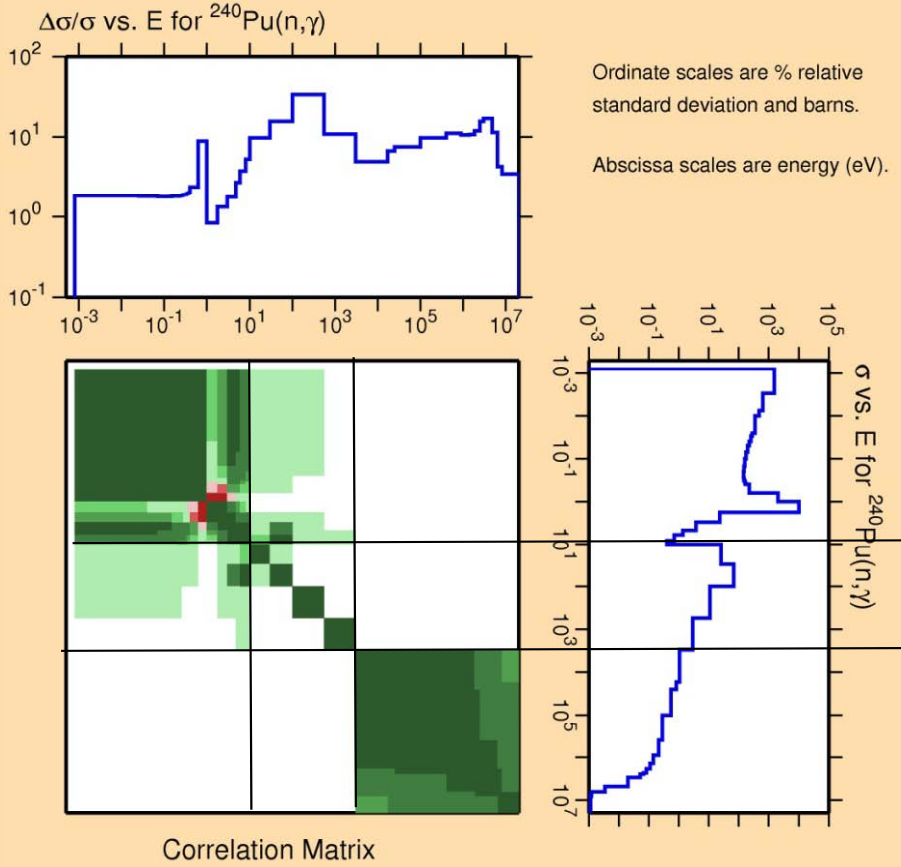






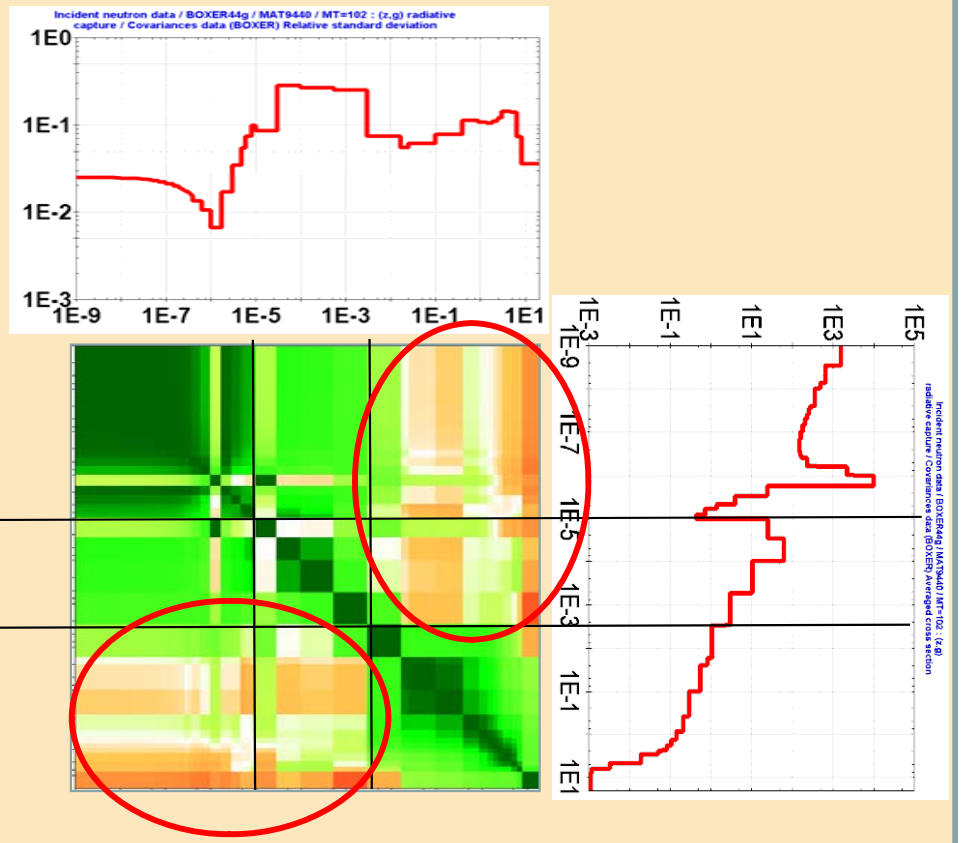
^{240}Pu(n,γ) Covariance Matrix in 44g

TENDL2010/ENDF



There is an overlap between the URR and the fast range (the URR goes from 5.7 keV to 40 keV and the fast range start at 5.7 keV).

TENDL2010/RANDOM EAF files



Can this effect explain part of the differences between TMC (using random fiels) and S/U methodologies (using ENDF covariances)?